Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.81e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 4.76e-01

Nearest Neighbors from the Training Set

Image not found
1-Naphthylamine
Measured: 4.00e-01
Predicted: 9.37e-04

Image not found
2-Butanone, 1-bromo-
Measured: 1.26e-01
Predicted: 7.89

Image not found
Dichloromethylphenylsilane
Measured: 1.96e-02
Predicted: 7.56e-01

Image not found
4-(2,4-Dinitroanilino)phenol
Measured: 3.43e-02
Predicted: 1.31e-11

Image not found
2,6-Diethylaniline
Measured: 1.59e-05
Predicted: 2.02e-02